Thermodynamics of the t-J Ladder: A Stable Finite Temperature Density Matrix Renormalization Group Calculation

Beat Ammon [1,2,3*], Matthias Troyer [2,3†] T.M. Rice [2] and N. Shibata[4]
1 *SCSC, Eidgenössische Technische Hochschule, CH-8092 Zürich, Switzerland*
2 *Theoretische Physik, Eidgenössische Technische Hochschule, CH-8093 Zürich, Switzerland*
[3] *ISSP, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan*
[4] *Institute of Applied Physics, University of Tsukuba, Ibaraki 305-3006, Japan*

Accurate numerical simulations of a doped t-J model on a two-leg ladder are presented for the particle number, chemical potential, magnetic susceptibility and entropy in the limit of large exchange coupling on the rung using a finite temperature density matrix renormalization group (TDMRG) method. This required an improved algorithm to achieve numerical stability down to low temperatures. The thermal dissociation of hole pairs and of the rung singlets are separately observed and the evolution of the hole pair binding energy and magnon spin gap with hole doping is determined.

Standard quantum Monte Carlo methods for the simulation of fermions are limited to relatively high temperatures due to the fermion sign problem. The density matrix renormalization group method (DMRG) [1] allows simulations of large clusters but is limited to groundstate properties. In this Letter we report on a finite temperature DMRG (TDMRG) [2,3] method using an improved numerically stable algorithm to simulate a strongly interacting fermion system down to low temperatures.

The TDMRG method applies the DMRG to the quantum transfer matrix (QTM) in the real space direction [4]. In the TDMRG iterations the QTM is enlarged in the imaginary time direction and iterates to lower temperatures at fixed Trotter time steps $\Delta\tau$. This is in contrast to the DMRG method in which the system grows in the real space direction. The TDMRG has the advantage that the free energy and other thermodynamic quantities for the *infinite* system can be obtained directly from the largest eigenvalue and the QTM and of the corresponding eigenvector.

The system we examine is a two-leg t-J ladder model in the limit where the exchange interaction across the rungs (J') is large compared to the value along the legs(J) and to the isotropic hopping integral t. The ground state properties of this model at low hole doping have been analyzed previously by exact diagonalization of small clusters [5,6]. In this limit $J' \gg J, t$ the thermal dissociation of hole pairs and the excitation of triplet magnons can be distinguished. These strong coupling processes are a good test for any method.

In this Letter we present accurate results for the magnetic susceptibility χ, the particle number n and the entropy density s in the grand canonical ensemble as a function of chemical potential μ and temperature T and then remap $\chi(\mu, T) \rightarrow \chi(n, T)$ to obtain the T-dependence at constant density.

Previous versions of the TDMRG method for fermions [3] have suffered from numerical instabilities due to the non-Hermiticity of the QTM and the corresponding density matrices which are constructed from the right and left eigenvector of the largest eigenvalue of the QTM. These numerical instabilities grow as the number of states kept is increased or the filling is changed away from half-filled bands. We have identified the loss of biorthonormality between the left and right eigenvectors $(v_i^{(l)}, v_j^{(r)}) = \delta_{ij}$ of the density matrix as the source of the problem. The biorthogonal but normalized eigenvectors $v_i^{(l)}/||v_i^{(l)}||_2$ and $v_j^{(r)}/||v_j^{(r)}||_2$ have to be multiplied with a factor $\left[(v_i^{(l)}, v_i^{(r)})/(||v_i^{(l)}||_2||v_i^{(r)}||_2)\right]^{-1/2}$, to become *biorthonormal*, which leads to severe loss of precision due to roundoff errors if the overlap between these vectors is small. These near-breakdowns occur especially often in conjunction with the second numerical problem, spurious small imaginary parts of (nearly) degenerate eigenvalue pairs. This latter problem can be solved by using the real and imaginary components of the corresponding complex conjugate eigenvector pairs and discarding the imaginary part of the eigenvalues, which are artifacts of roundoff errors and are only of the order of the machine precision. To circumvent the loss of precision in the former problem of nearly orthogonal eigenvectors our algorithm uses an iterative re-biorthogonalization step [7] for the eigenvectors kept, which stabilizes the method for all temperatures. Technical details of the algorithms will be presented elsewhere [8]. In Tab. I we show results of numerical stability tests of the original [2,3] and our improved algorithm for the case of noninteracting spin $S = 1/2$ fermions in one dimension. For this simple fermionic model the original TDMRG method becomes numerically unstable whenever more than about $m = 10$ states are kept, thus severely restricting the achievable accuracy. The improved algorithm presented here, on the other hand, is always numerically stable and achieves much higher accuracy. The test example clearly demonstrates the need for numerical stabilization in the simulation of fermionic models.

The results of the stabilized TDMRG method are accurate and unbiased, with errors only originating from the

TABLE I. Free energy density f for noninteracting spin $S = 1/2$ fermions on a chain with $\mu = 0$ at a temperature $T = 0.1$ after a hundred DMRG steps ($\Delta\tau = 0.1$), where energies are given in units of the hopping integral t. The first column (I) is the original TDMRG algorithm [2,3], and the second column (II) is our improved method including the re-biorthogonalization step. Cases where the algorithm becomes numerically unstable are denoted with $\dagger n$, where n is the number of DMRG steps that could be performed successfully.

algorithm	I	II
$m = 10$	-0.65500	-0.65500
$m = 20$	† 16	-0.67225
$m = 30$	† 39	-0.67413
$m = 40$	† 9	-0.67441
$m = 50$	† 7	-0.67454
$m = 60$	† 50	-0.67457
$m = 80$	† 8	-0.67462

finite size of the Trotter time steps and the truncation in the DMRG algorithm. The latter are usually very small if the number of states kept, m, is large enough, and the former can be eliminated by extrapolating $\Delta\tau \to 0$ by fitting to a polynomial in $\Delta\tau^2$. We have used Trotter time steps from $\Delta\tau t = 0.01$ to $\Delta\tau t = 0.2$, and m between $m = 40$ and $m = 60$. We made use of spin conservation symmetry, the subspace of zero winding number and the reflection symmetry of the ladder along the rungs to optimize the calculations and reduce numerical errors.

Thermodynamic quantities such as the internal energy U, the hole density $n_h(= 1-n)$ and the magnetic susceptibility χ have been determined directly from the eigenvectors of the transfer matrix [4,9]. This is preferable to taking numerical derivatives of the free energy density obtained from the largest eigenvalue of the QTM.

The low temperature properties of a doped t-J two-leg ladder in the limit $J' \gg J, t$ are determined solely by the singlet hole pairs (HP) [5]. They form a hard core boson gas with a bandwidth of $4t^*$, with $t^* = 2t^2(J' - 4t^2/J')^{-1}$ in second order perturbation theory. Neglecting a weak nearest neighbor attraction, the HP fluid can be mapped to an ideal Fermi gas in this one dimensional geometry. As the temperature T is increased the HPs dissociate into two quasiparticles (QP), each consisting of a single electron with spin $S = 1/2$ in a rung bonding state. Each QP propagates with a bandwidth of $2t$ so that in the limit of low hole doping $n_h \ll 1$ the HP binding energy is $E_B = J' - 4t + 4t^2(J' - 4t^2/J')^{-1}$. The gas of QPs with density $n_{QP}(T)$ contributes to the spin susceptibility as a nondegenerate gas of $S = 1/2$ fermions. A second contribution comes from the thermal excitation of singlet rungs to a triplet magnon state. The activation energy for a magnon Δ_M ($= J' - J + J^2/2J'$ in second order perturbation theory in the limit $n_h \to 0$ [10]) is larger than that of the QPs ($\Delta_{QP} = E_B/2$) but since the density of

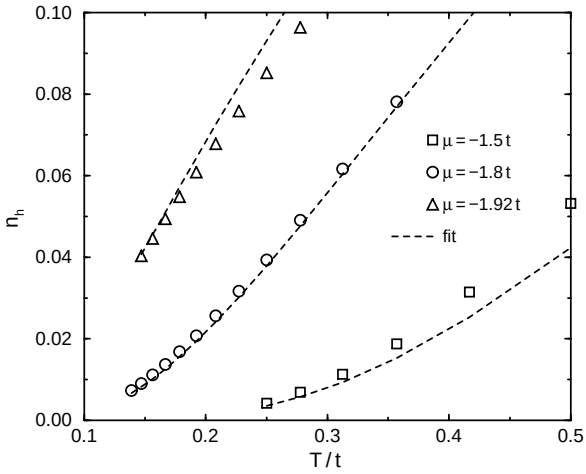

FIG. 1. Hole density n_h as a function of electron chemical potential μ and temperature T in the strong coupling regime $J = t/2 = J'/10$. The dashed lines are fits to a hard core boson model for the hole pairs. Note, the HP chemical potential is -2μ.

QPs is limited by the hole density ($n_{QP}(T) \leq n_h$), the temperature evolution of $\chi(n, T)$ is determined largely by the magnons at low doping.

We now turn to the presentation of our finite temperature results obtained using the improved TDMRG algorithm for $J = t/2 = J'/10$ and compare them to expectations based on the above discussion of this strong coupling regime. As the calculations were performed in the grand canonical ensemble we first present results for the hole density $n_h(\mu, T)$. A selection of our results is presented in Fig. 1 including a fit to a hard core boson model for the HPs:

$$\epsilon^k_{HP} = \epsilon_{HP} + 2t^* \cos k + 2\mu n_h. \qquad (1)$$

Fitting the data for $n_h < 0.1$ at temperatures $T < 0.5t$ we obtain an estimate for the center of the band for HPs at $\epsilon_{HP} = 4.82(6)t$ and a bandwidth $4t^* = 1.5(2)t$. The minimum energy to add a HP to an undoped ladder is $\epsilon_{HP} - 2t^* = 4.1(1)t$, in good agreement with values from the finite clusters ($\epsilon_{HP} \approx 4.71t$, $4t^* \approx 1.494t$ [5]).

A further confirmation of the validity of this hard core boson model for the HPs comes from considering the low temperature entropy density per site s, determined from the free energy density f and the energy density u as $s = (u - f)/T$. As can be seen in Fig. 2 the entropy at $T < 0.3t$ and low doping ($n_h < 0.1$) is also well described by the hard core boson model for the HPs.

At higher temperatures the thermal dissociation of HPs into two independent QPs and the thermal excitation of magnons from rung singlets govern the thermodynamics. These processes show up in the spin suscep-

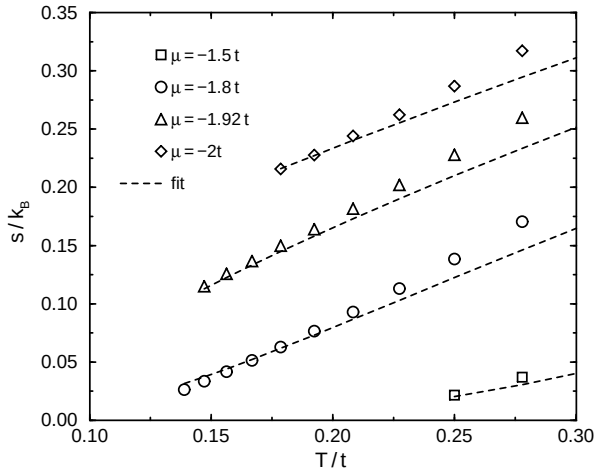

FIG. 2. Entropy density s as a function of chemical potential μ and temperature T in the strong coupling regime $J = t/2 = J'/10$. The dashed lines are the values for the same hard core boson model as in Fig. 1, using the parameters obtained in that fit.

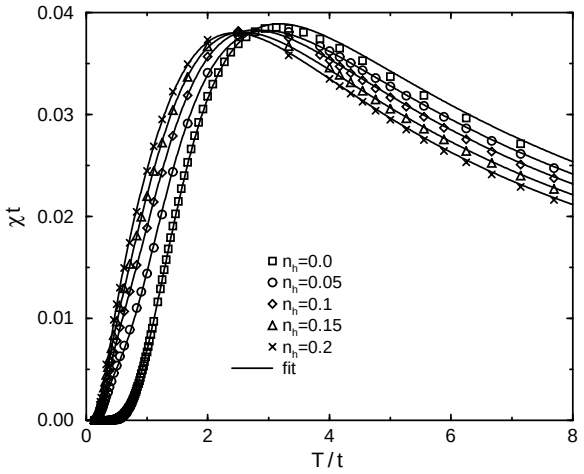

FIG. 3. Uniform magnetic susceptibility per site χt of the t-J ladder for $J = t/2 = J'/10$ and different hole-densities n_h. The symbols denote the results of the TDMRG algorithm, and the solid lines are the fitted curves according to Eq. (2). The fitting parameters are listed in Tab. II.

tibility $\chi(T)$, which is easiest to interpret in the canonical ensemble with fixed hole density n_h. Therefore we use $n_h(\mu, T)$ to remap $\chi(\mu, T) \rightarrow \chi(n_h, T)$. The values of $\chi(\mu, T)$ were calculated by measuring the magnetization $\langle S^z(T)\rangle$ in the presence of a small external field $h/t = 5\times10^{-3}$. The results for $\chi(n_h, T)$ appear in Fig. 3.

At high temperatures $T \gg J'$, χ follows a Curie-law for free spins $\chi = (1 - n_h)/4T$, and it decreases when the temperature is lowered below the magnon-gap $\Delta_M \approx 4.13t$. The maximum of the peak is shifted towards lower T with increasing doping, indicating a reduction of the magnon gap due to interactions with holes. Simultaneously the magnon bandwidth is enhanced, indicating that the energy of a localized magnon is not much changed by the holes. At very low temperatures of $T < 0.5t$ we can see a second exponential decrease of χ with a smaller gap, which we attribute to the recombination of QPs into HPs at temperatures below the QP-gap, $\Delta_{QP} = E_B/2$. Note the magnitude of this contribution increases with n_h.

A quantitative description of $\chi(n_h, T)$ can be given by adding separately the contributions of the QPs χ_{QP} and of the magnons χ_M, i.e.:

$$\chi(n_h, T) = \chi_{QP}(n_h, T) + \chi_M(n_h, T). \tag{2}$$

χ_{QP} is approximated by the value for free spins $\chi_{QP} = n_{QP}(T)/4T$ with a temperature dependent density of the QPs determined by the energy dispersion of the QPs $\varepsilon^k_{QP} = \Delta_{QP} + a_{QP}(1 + \cos k)/2$ with $\beta = 1/T$:

$$n_{QP} = \frac{n_h}{\pi}\int_{-\pi}^{\pi} dk\, \frac{1}{e^{\beta\varepsilon^k_{QP}} + 1}. \tag{3}$$

TABLE II. Gap of the spin $S = 1/2$ quasi-particles Δ_{QP} and magnon gap Δ_M, as well as the parameters a_{QP} (a_M) which determine the bandwidth of the quasi-particles (magnons) obtained by fitting Eq. (2) to our TDMRG data for different hole densities n_h.

n_h	Δ_{QP}	Δ_M	a_{QP}	a_M
0.0	-	4.1(1)	-	0.7(1)
0.025	0.7(1)	3.4(1)	0.9(2)	1.6(2)
0.05	0.8(1)	3.3(1)	0.9(2)	1.8(2)
0.1	1.0(1)	3.3(1)	0.6(3)	1.7(2)
0.15	0.9(1)	3.2(1)	1.3(2)	2.0(2)
0.2	0.9(1)	3.2(1)	1.4(2)	2.0(2)

The density of rungs occupied by two spins at low temperatures where all holes are bound in HPs is $1 - n_h$ but exciting QPs reduces the number of such rungs by one for each QP so that the rung density is then $1-n_h-n_{QP}$. Our approach to a model for χ_M is simply to scale the form for undoped ladders proposed by Troyer *et al.* [9] by this two-spin rung density leading to

$$\chi_M = (1 - n_h - n_{QP})\beta\frac{z(\beta)}{1 + 3z(\beta)}, \tag{4}$$

where $z(\beta) = \int_{-\pi}^{\pi} dk(2\pi)^{-1}\exp(-\beta\varepsilon^k_M)$, and $\varepsilon^k_M = [\Delta_M^2 + 4a_M(1 + \cos k)]^{1/2}$ [11].

The parameters obtained by a fit of this model to the TDMRG data are shown in Tab. II. The main change upon doping is the decrease of the magnon gap Δ_M [10,12,13] due to interactions between the magnons and

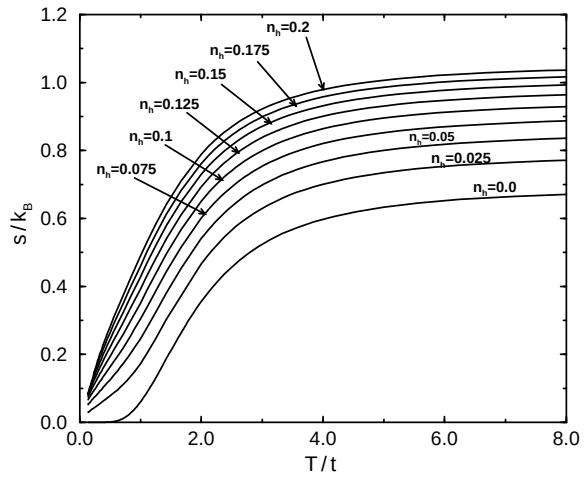

FIG. 4. Entropy density of the doped t-J ladder with $J = t/2 = t'/2 = J'/10$ and different hole-densities n_h.

QPs. Due to hybridization with higher lying bands the QP bandwidth a_{QP} is also reduced from the leading order perturbation result $a_{QP} = 2t$, but the QP gap Δ_{QP} is in reasonable agreement with the second order perturbative estimate of $0.98t$. The increase of Δ_{QP} (or equivalently the binding energy E_B) with n_h, can be attributed to an effective repulsion between the QPs and HPs. A similar increase of the QP gap Δ_{QP} was found in Ref. [12]. This is an issue which warrants further investigations.

Finally, in Fig. 4 we show the entropy density s, remapped in the same way to the canonical ensemble of fixed n_h. In the limit of $T \to \infty$ $s_\infty = (1 - n_h)\ln 2 - n_h \ln n_h - (1 - n_h)\ln(1 - n_h)$. At $T/t = 20$ the entropy has acquired between 99.4% of its maximal value s_∞ for $n_h = 0.025$ and 99.7% for $n_h = 0.2$. Below the magnon gap Δ_M, the entropy decreases exponentially, for the undoped Heisenberg ladder down to $s = 0$. In the presence of hole doping, the exponential decrease shows a crossover to a linear decrease at low temperatures, as is expected for Luther-Emery liquids. This behavior is consistent with the hard core boson model proposed for the magnons. Quantitative fits are however better performed on $s(\mu, T)$, as we did earlier, due to added uncertainties arising from the remapping to constant hole doping.

In conclusion, we have developed the first numerically stable TDMRG algorithm for fermionic systems. This has enabled us to calculate accurate results for the magnetic susceptibility χ and the entropy density s of the doped t-J ladder with strong exchange on the rungs down to low temperatures in the thermodynamic limit of infinite system size. The system we have studied has two crossovers as the spins bind in singlet pairs and the holes in hole pairs. These crossovers can be clearly seen in the numerical data and demonstrate that this form of the TDMRG can be successfully used to reliably simulate strongly interacting fermions over a wide temperature range.

Finally, very recently Rommer and Eggert report TDMRG calculations for a spin chain with impurities [14] which uses the same method as we do to overcome the problems caused by complex eigenvalues, but they did not introduce the re-biorthogonalization which for fermionic models, we find is essential.

We wish to thank E. Heeb, M. Imada, and X. Wang for useful discussions. Most of the calculations have been performed on the DEC 8400 5/300's of the C4-cluster at ETH Zürich.

* present address: Institute for Solid State Physics, University of Tokyo, Roppongi 7-22-1, Tokyo 106, Japan.

† present address: Theoretische Physik, Eidgenössische Technische Hochschule, CH-8092 Zürich, Switzerland.

[1] S.White, Phys. Rev. Lett. **69**, 2863 (1992); S. White, Phys. Rev. B **48**, 10345 (1993).

[2] R.J. Bursill, T. Xiang, and G.A. Gehring, J. Phys. Cond. Matt. **8**, L583 (1996); X. Wang and T. Xiang, Phys. Rev. B **56**, 3177 (1997); N. Shibata, J. Phys. Soc. Jpn. **66**, 2221 (1997); T. Xiang, preprint cond-mat/9808179; K. Maisinger and U. Schollwöck, Phys. Rev. Lett. **81**, 445 (1998).

[3] N. Shibata, B. Ammon, M. Sigrist, M. Troyer, and K. Ueda, J. Phys. Soc. Jpn. **67**, 1086 (1998); T. Xiang, Phys. Rev. B **58**, 9142 (1998); T. Mutou, N. Shibata, and K. Ueda, Phys. Rev. Lett. **81**, 4939 (1998) N. Shibata and K. Ueda, preprint cond-mat/9808301.

[4] H. Betsuyaku, Prog. Theor. Phys. **73**, 319 (1985); T. Yokota and H. Betsuyaku, Prog. Theor. Phys. **75**, 46 (1986).

[5] M. Troyer, H. Tsunetsugu, and T.M. Rice, Phys. Rev. B **53** 251 (1996).

[6] For a review see E. Dagotto and T.M. Rice, Science **271**, 618 (1996).

[7] V. Simoncini, SIAM J. Matrix Anal. Appl. **18**, 419 (1997).

[8] B. Ammon and M. Troyer, in preparation.

[9] M. Troyer, H. Tsunetsugu, and D. Würtz, Phys. Rev. B **50**, 13515 (1994).

[10] M. Reigrotzki, H. Tsunetsugu, and T.M. Rice, J. Phys. Cond. Matt. **6**, 9235 (1994).

[11] S. Gopalan, T.M. Rice, and M. Sigrist, Phys. Rev. B **49**, 8901 (1994).

[12] D. Poilblanc, D.J. Scalapino, and W. Hanke, Phys. Rev. B **52**, 6796 (1995).

[13] D. Poilblanc, H. Tsunetsugu, and T.M. Rice, Phys. Rev. B **50**, 6511 (1994); R.M. Noack, S.R. White, and D.J. Scalapino, Phys. Rev. Lett. **73**, 882 (1994).

[14] S. Rommer and S. Eggert, preprint cond-mat/9812001.